A microscopic model of resonant double-barrier tunneling in a quantum system

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A simple model of resonant electronic transport through a double-barrier structure was developed. For each region of the system, analytic solutions to Schrödinger's equation were obtained, and these solutions formed the basis of the Matlab code written to output plots of resonant peaks based on varying barrier parameters. Resonances in transmission probability and in the electron density inside the quantum well were then considered for a number of these different parameters. Also, equilibrium and non-equilibrium cases were modeled for the same set of parameters; the observed behavior was somewhat dissimilar. As an application of the model to device physics, a brief discussion of the concepts governing resonant tunneling diodes is also included.

A familiar fact in the realm of physics is that on very small size scales, some of the tidiness of the classical, macroscopic world collapses into that of quantum mechanics. This certainly holds true for sizes on the order of magnitude of fractions of nanometers—the size of a Bohr radius. In this quantum domain, we consider the wave nature of the electron to describe its interaction with a series of potential barriers. The model developed is a simple one: a one-dimensional, piecewise-constant system consisting of two square barriers. Nonetheless, this model does demonstrate a number of interesting features and may be extended to any length series of quantum wells.

My project was to develop code in Matlab to simulate the behavior of electrons tunneling through a double-barrier structure. Two features form the basis of the behavior of the model: transmission probability and well density. From a consideration
of the transmission probabilities for a number of different electron energies, we calculate the current through the two barriers. From a comparable consideration of density as a function of incident energy, we calculate the total density of electrons inside the quantum well.

**BACKGROUND & THEORY**

To introduce the situation, first consider the typical problem of a particle in a one-dimensional box. The behavior of the particle—say, an electron—in this situation follows from the solution of Schrödinger’s equation in one dimension, which gives rise to \( n \) discrete energy levels with \( n^2 \) spacing. As long as this idealistic box has infinite walls, the electron’s wavefunction will be zero outside the box and purely sinusoidal inside. If, though, this box is modified so as to have walls of finite height, the particle has a chance to escape from, or tunnel out of, the confining potentials. High potentials relative to the energy of the particle, and, likewise, wide walls compared to the width of the well, correspond to less chance of escape, and hence a longer lifetime of the box’s “bound” eigenstate.

Now, instead of picturing a particle sitting inside such a potential well, consider a coherent beam of electrons projected upon two such barriers of finite height and width, with the energy of the electrons lower than that of the barriers (see Fig. 1). In this one-dimensional picture, when the

![FIGURE 1. Diagram of the series of potential barriers defining the parameters used.](image-url)
incident flux encounters a potential barrier, it has only two options: reflection or transmission. The probability of transmission through the series of barriers peaks sharply at particular incident energies. The exact energy of these resonant modes depends on the height and width parameters\(^1,2\) describing the barriers and on the length of the well between them.

Obtaining the transmission coefficients themselves involves matching the solutions, for each region of interest, to the one-dimensional, time-independent Schrödinger equation in position space:

\[
\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x) \tag{1}
\]

where \(m\) is the mass of the electron, and \(\hbar = 1.055 \cdot 10^{-27}\) in cgs units \([1]\). We are assuming a piecewise constant potential in this model. In those regions where \(V(x) = 0\), the equation simplifies to

\[
-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi
\]

\[
\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi \tag{2}
\]

where \(k = \sqrt{\frac{2mE}{\hbar^2}}\). We thus have a second-order differential equation to which the two linearly independent solutions are purely oscillatory, and hence the general solution may be written as \(\psi(x) = A\sin(kx) + B\cos(kx)\), or, more conveniently for our purposes, \(\psi(x) = Ae^{ikx} + Be^{-ikx}\). Similarly, for a nonzero constant potential of magnitude \(V_0\), Schrödinger’s equation becomes

\[\text{1 All Matlab code is included in Appendix B}\]
\[\text{2 See Appendix B, parameters.m}\]
\[- \frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = (E - V_0) \psi \]
\[
\frac{d^2 \psi}{dx^2} = - \frac{2m(E - V_0)}{\hbar^2} \psi = q^2 \psi
\]

with \( q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \), assuming \( E < V_0 \) as is the case for the barriers here [1]. For this case, the two linearly independent solutions are rising and falling exponentials and the corresponding general solution is \( \psi(x) = Ce^{\alpha x} + De^{-\alpha x} \). Considering all the regions of the given model, then, and assuming that \( V_m < E \), we have

\[
\psi(x) = \begin{cases} 
Ae^{ikx} + Be^{-ikx}, & x < a \\
Ce^{ax} + De^{-ax}, & a < x < b \\
Fe^{ikx} + Ge^{-ikx}, & b < x < c \\
He^{mx} + Le^{-mx}, & c < x < d \\
Je^{ikx} + Ke^{-ikx}, & x > d 
\end{cases}
\]

here defining \( q = \sqrt{\frac{2m(V_1 - E)}{\hbar^2}} \) and \( p = \sqrt{\frac{2m(V_2 - E)}{\hbar^2}} \) so as to explicitly allow the left and right potential barriers to have different magnitudes.

The last idea that we need to develop in order to calculate the transmission coefficients through our series of barriers is that of probability current. Briefly stated, we can think of the probability of finding an electron in a particular spatial region changing due to a probability flow, or current, entering or leaving that region. This current we define as \(^3\)

\[
j_x = \frac{\hbar}{2mi} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)
\]

where \( \psi^*(x) \) is the complex conjugate of the wavefunction \( \psi(x) \).

\(^3\) For a derivation of the probability current from Townsend, see Appendix A
Finally, we define the transmission coefficient as $T = \frac{j_{\text{trans},x>d}}{j_{\text{inc},x<a}}$ [1]. Since in our model the potential before and after the series of barriers is the same—namely, $V=0$ for both $x < a$ and $x > d$—$T$ simplifies to a ratio of the squared moduli of the corresponding coefficients from the original wavefunctions:

$$T = \frac{|H|^2}{|A|^2} \quad \text{for electrons incident from the left (+k states), and}$$

$$T = \frac{|B|^2}{|K|^2} \quad \text{for electrons incident from the right (-k states).} \quad (6), (7)$$

These unknown variables become numerically meaningful by satisfying the necessary boundary conditions—namely, that the wavefunctions and their first derivatives be continuous across each interface. These conditions generate two equations per boundary, or four per barrier. Thus, for our system of two barriers, we must thus satisfy eight boundary equations. To solve such systems analytically poses a straightforward but algebraically daunting undertaking, even for a single barrier. This, then, is where Matlab enters the picture.

The attached Matlab m-file resonant.m calculates the probability of transmission for a single input energy. To demonstrate the $n^2$-dependence of the resonant energy levels, we plot these transmission coefficients for many different energies and note the location of the peaks. Generally speaking, if the two barriers are symmetric—having equal widths and equal heights—then the probability of transmission through both barriers at resonance approaches 100%. The higher the barriers are, the more like delta functions the transmission peaks become. Another way to think of this
feature is in terms of filters: tall barriers are more selective of the energy of electrons that they will let through than lower barriers. Another general characteristic is that the first resonant peak occurs at a lower energy for wider wells than for narrow ones (see Fig. 2).

To understand this statement, consider that the uncertainty in position of a particle in a very narrow well is less than the uncertainty for one in a wide well. To compensate for this and obey the constraints of Heisenberg’s notorious uncertainty principle, the allowed momenta—and hence energies—of the more confined particle are greater than the corresponding momenta and energies of a particle in a wider well. As one physics professor once described, “A particle does not like to live in a narrow potential well.” [2]

A peak in transmission probability means that the number of electrons tunneling through the barriers achieves a relative maximum. We define the minimum incident energy as $\varepsilon_{\text{min}}$ and the maximum incident energies (one for the $+k$ and one for the $-k$ states) $\mu_L$ and $\mu_R$ (also known as the electrochemical potentials, or quasi-Fermi levels).

\[^4\text{See Appendix B}\]
By integrating all the probabilities of transmission over this energy range of interest \((\varepsilon_{\min} < E < \mu_{L,R})\), we obtain the current through the structure:

\[
J_{I,\tau} = \int_{\varepsilon_{\min}}^{\mu_{L,R}} T(E) dE
\]  

(8)

If the transmission peaks were true delta functions, the current would be a step function, with one step at every resonance. Electrons that penetrate the potential barriers at these resonant energies populate the space inside the well; therefore, a maximum in the density of electrons in the well occurs for every maximum probability in transmission. We may in fact call this density the probability density, and define the quantity \(dx|\psi(x)|^2\) as the probability of finding the electron between \(x\) and \(dx\), where \(\psi(x)\) describes the electron’s wavefunction inside the well. For a single energy, then, we obtain the well density\(^5\) \(n(E)\) by integrating from \(x = b\) to \(x = c\):

\[
n(E) = \int_{b}^{c} dx|\psi(x)|^2
\]  

(9)

Repeating this procedure for a number of \(k\) values reveals peaks in the same locations as the transmission resonances, as expected.

The shape of the transmission and density peaks themselves fit Lorentzian functions, of the form

\[
L(E) = \frac{\Gamma^2}{(E - E_{\text{res}})^2 + \left(\frac{\Gamma}{2}\right)^2}
\]  

(10)

where \(\Gamma\), describing the half-width of the peak, is a parameter related to the "escape frequency" of an electron in the well [3]. This frequency is greatest for electrons closest to the relevant electrochemical potential \(\mu_L\) or \(\mu_R\), and so the peaks are widest for these
higher energies. Thus, as Fig. 1 demonstrates for the transmission peaks, the broadest peaks correspond to the highest resonant modes.

Any nonzero density of electrons inside the well implies a Coulomb interaction between the “bound” particles, generating a repulsive potential that interacts with the existing well depth. Before we consider the interaction itself, though, we must calculate the density contribution from every $k$ value incident upon the system. We determine this total density\(^6\) by taking the integral of all the individual $n$ values with respect to energy, up to the given electrochemical potential:

$$N = \int_{E_{\text{min}}}^{E_{\mu}} n(E)dE$$

The well potential $V_m$ rises linearly as a function of this density according to the expression

$$V_m = V_0 + c \cdot N$$

where $c$ is a constant that may characterize the properties of the particular material or source of the potential barriers, and $V_0$ is the well height before considering any Coulomb interactions. Accounting for this dynamic potential, however, complicates the situation in a nontrivial manner. As the depth of the well decreases, the electronic wavefunctions change and resonance locations increase accordingly. As the energy of each resonant level increases, the highest modes will simply “pop out” the top of the well, and the wavefunctions will adjust to the newly perceived potentials (see Fig. 3). This alteration of the density of electrons inside the new well changes the well depth, which changes the effective density, and so the picture continues. The issue then

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5 See Appendix B, \texttt{readens.m}
6 See Appendix B, \texttt{nvsvm.m}
becomes a matter of determining a self-consistent model for this system—that is, finding its stable points of operation.

**RESULTS**

We had expected that as the well potential increases and pushes out resonant modes, the electron density would simply decrease. The observed case proved somewhat less obvious than this. If both the $+k$ and the $-k$ electrons are filled to the same chemical potential (from Fig. 1, if $\mu_L = \mu_R$), then there is a true Fermi level $E_f$ for the system—namely, $E_f = \mu_L = \mu_R$. The location of the transmission peaks in this double-barrier system depends on the parameters of both the barriers; switching the parameters of the first and second barriers has no effect on the tunneling probability. Thus, if $\mu_L = \mu_R$, 

![Graph](image.png)

FIGURE 3. As the height of the potential well increases, the locations of the resonant levels increase accordingly.
exactly the same number of electrons tunnels through the barriers from the left as from the right, so we obtain no net current through the system.

If we plot the individual +k or -k currents individually, or the total, integrated density \( N \) as a function of \( V_m \), we find that the levels actually increase initially, then decrease smoothly as expected (see Fig. 4). This feature we explain by recalling two previously mentioned characteristics: firstly, that the width of the resonant peaks (for \( T \) and for \( n \) alike) increases as the electron's energy increases, such that the highest modes have the broadest peaks; secondly, that as the depth of the potential well decreases, the locations of resonant energies increase accordingly. As we integrate \( T \) and \( n \) to obtain \( J \) and \( N \), respectively, we thus obtain current and density contributions from broader and broader peaks as \( V_m \) increases. When the increasing height of the well finally does push out a resonant level completely, we

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure4.png}
\caption{Plots for a 6.5 Å well. (a) The total density decreases smoothly as a function of the well potential. (b) The current for left-going and right-going electrons is equal, so there is no net current at equilibrium.}
\end{figure}
correspondingly observe a significant drop in the current and total density. This increase-then-decrease behavior repeats until no resonances remain in the well, at which time the levels simply decrease.

For the non-equilibrium case, we cannot discuss a true Fermi level of the system, but we can discuss the local quasi-Fermi levels $F^+ = \mu_L$ and $F^- = \mu_R$ [3]. When these two are not equal, the behavior of the integrated density and currents proves slightly more complicated than at equilibrium. Namely, the number of “bumps” in the curve increases with well length, a direct result of the fact that there we only have local, quasi-Fermi levels and not one true one for this non-equilibrium situation. For each bulge in the equilibrium plots, we find two for non-equilibrium, corresponding to the differing contributions from the two unequal electrochemical potentials.

The total number of protrusions, for equilibrium and non-equilibrium alike, depends on the length of the quantum well (see Fig. 5). This result follows from the previous consideration that longer well lengths correspond to modes of lower energies, such that the number of resonant peaks in the longer wells is greater than that for the shorter ones even as $V_m$ increases. The self-consistent operating point of the system occurs where we can satisfy Eq. (12)—graphically, where plot of $N$ vs. $V_m$ and $V_m$ vs. $V_m$ would intersect.

In all this Matlab modeling, we did not come away wholly unscathed from the specter of numerical inconsistencies. In particular, a close inspection of Fig. 5 reveals very small oscillations most pronounced when $V_m$ is close to zero. These pesky oscillations are a consequence of the sharpness of the first resonant peak and the finiteness of the energy increment over which we integrate to obtain the current and
total density. Matlab works very well with matrices and not as well with continuous variables, such as we would ideally have the allowed incident energies. We use the trapezoidal method of integration in the actual Matlab calculations. However, since the

FIGURE 5. The behavior of the density and current becomes more complex as length of the quantum well increases. Plots of density and current shown are for well lengths of (a,b) 4, (c,d) 6.5, and (e,f) 9 angstroms.
first resonant peak is extremely sharp—sharpest for low \( V_m \) values—we sample a relatively small number of points in this first peak. The height of this peak itself thus does not consistently and accurately represent the true theoretical value, and we see an oscillation in the height of the peaks with a period exactly equal to the increment of energy used set in the code parameters. Smaller energy increments, though, correspond to more accurate sampling of the resonant peaks; therefore, the amplitude and range of the oscillations becomes markedly smaller for even a change of a factor of five in the energy step size. On the other hand, the computational speed slows down just as noticeably.

**APPLICATIONS**

So far, we have discussed a number of features of this double-barrier system without really considering the actual, physical source of the potentials, or the possible applications of such a system. We now turn our considerations in this direction and to a mesoscopic size scale to discuss briefly resonant tunneling diodes, whose basic principles of operation rely on the type of model we have just described. The operation of most mesoscopic conductors depends on the formation of a very thin conducting layer of electrons formed at a \( pn \)-junction like AlGaAs/GaAs. In layers of this nature, electrons flow laterally along the heterojunctions [3]. In resonant tunneling diodes, however, current flows transversely to the thin layer, in a “vertical” configuration (see Fig. 6).
We may think of the structure as a filter permitting only electrons of a particular energy transmit, as mentioned earlier. When we apply a bias voltage, we lower the resonant energies relative to the incident energies of the electrons from the emitter (here, the top layer of GaAs). If we continue to increase the applied voltage past some threshold level $V_T$, the resonant level falls below the range of the emitter’s incident energies—in other words, the energy level of the resonance is below that of the conduction band in the emitter. Since the filter energy is lower than that of the conduction band, a bias exceeding this threshold voltage effects a sharp drop in the observed current. At this point, the system exhibits a negative differential resistance [3].

**Conclusions**

Although the model we considered in this project comprises a number of significant physical simplifications, we have thoroughly understood it and have demonstrated numerically some general, known features of double-barrier tunneling, such as the behavior of the resonances, as well as some less-anticipated ones like the
shape of the $N$ vs. $V_m$ curves. Further efforts to relax some of the assumptions used in the development of this model certainly suggest a route of future code development.

ACKNOWLEDGEMENTS

I would like to extend many thanks to Dr. Selman Hershfield, my research mentor, for all of his efforts this summer. Thanks are also in order for Drs. Kevin Ingersent and Alan Dorsey, the director and associate director of the physics Research Experience for Undergraduates (REU) program at the University of Florida, and Darlene Latimer, whose coordination efforts facilitated this program. I also make a grateful mention of the National Science Foundation for its sponsorship of these summer REU programs.
To see how the probability current arises, consider \( \frac{\partial \psi^* \psi}{\partial t} \), the time rate of change of the probability density. Using the time-dependent Schrödinger equation, we see that the time derivative of the wavefunction is given by

\[
\frac{\partial \psi(x,t)}{\partial t} = \frac{1}{i\hbar} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \right]
\]

Therefore

\[
\frac{\partial \psi^*(x,t)}{\partial t} = \frac{1}{-i\hbar} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*(x,t)}{\partial x^2} + V(x)\psi^*(x,t) \right]
\]

and

\[
\frac{\partial \psi^* \psi}{\partial t} = \psi \frac{\partial \psi^*}{\partial t} + \psi^* \frac{\partial \psi}{\partial t}
\]

\[
= \frac{\psi}{-i\hbar} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + V(x)\psi^* \right] + \frac{\psi^*}{i\hbar} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi \right]
\]

\[
= \frac{\psi}{-i\hbar} \left( -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} \right) + \frac{\psi^*}{i\hbar} \left( -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \right)
\]

This equation can be expressed in the form

\[
\frac{\partial \psi^* \psi}{\partial t} = -\frac{\partial j_x}{\partial x}
\]

where

\[
j_x = \frac{\hbar}{2mi} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)
\]

This reflects a local conservation law — of probability. For example, if we integrate between \( x = a \) and \( x = b \), we obtain
\[ \frac{d}{dt} \int_{b}^{a} dx \psi^* \psi = -j_x(b,t) + j_x(a,t) \]

If the net probability of finding the particle between \( a \) and \( b \) increases, it does so because of a net probability current flowing into the region either at \( a \) [positive current flows in the positive \( x \) direction and hence \( j_x(a,t) > 0 \) means inward flow at \( a \)] or at \( b \) [negative current means current in the negative \( x \) direction and hence \( j_x(b,t) < 0 \) means inward flow at \( b \)]. Thus the probability in a region of space increases or decreases because there is a net probability flow into or out of that region [1].
APPENDIX B: MATLAB M-FILES

parameters.m
resonant.m
resdens.m
resonantcomp.m
lengthen.m
nvsvm.m
%parameters.m
%created 29/06/01
%last modified 26/07/01

%Defines barrier parameters for resonant tunneling problem
%cgs units

hbar=(6.6260755/(2*pi))*10^-27; %units ergs
qe=1.60217733e-12; % (qe) ergs = 1eV
Emin=1e-14;
Einhr=1e-14;

a=0e-8; %x placement of first edge of first barrier
w1=.53e-8; %width of first barrier
L=9e-8; %length of well
w2=1.5*.53e-8; %width of second barrier
b=a+w1; %x placement of second edge of first barrier
c=b+L; %x placement of first edge of second barrier
d=c+w2; %x placement of second edge of second barrier

V1=15*qe; %height of first barrier
V2=15*qe; %height of second barrier

m=9.1093897*10^-28; %mass of electron
%resonant.m
%created 29/06/01
%last modified 26/07/01
%written by Shanna Crankshaw

%finds the transmission coefficient for one incident energy on a series
%of two
%square barriers
%finds the scattering matrix

k=sqrt(2*m*E/hbar^2);
q=sqrt(2*m*(V1-E)/hbar^2);
p=sqrt(2*m*(V2-E)/hbar^2);

ml=[exp(i*k*a) exp(-i*k*a); i*k*exp(i*k*a) -i*k*exp(-i*k*a)];
m2=[exp(q*a) exp(-q*a); q*exp(q*a) -q*exp(-q*a)];
m3=[exp(q*b) exp(-q*b); q*exp(q*b) -q*exp(-q*b)];
m6=[exp(p*c) exp(-p*c); p*exp(p*c) -p*exp(-p*c)];
m7=[exp(p*d) exp(-p*d); p*exp(p*d) -p*exp(-p*d)];
m8=[exp(i*k*d) exp(-i*k*d); i*k*exp(i*k*d) -i*k*exp(-i*k*d)];

m23=m2*inv(m3);
m23=[cosh(q*w1) (-1/q)*sinh(q*w1); -q*sinh(q*w1) cosh(q*w1)];

if E>Vm
    km = sqrt(2*m*(E-Vm)/hbar^2);
    m4=[exp(i*km*b) exp(-i*km*b); i*km*exp(i*km*b) -i*km*exp(-i*km*b)];
    m5=[exp(i*km*c) exp(-i*km*c); i*km*exp(i*km*c) -i*km*exp(-i*km*c)];
    m45=m4*inv(m5);
m45 = [cos(km*L) (-1/km)*sin(km*L); km*sin(km*L) cos(km*L)];
elseif E<Vm
    km = sqrt(2*m*(Vm-E)/hbar^2);
    m4=[exp(km*b) exp(-km*b); km*exp(km*b) -km*exp(-km*b)];
    m5=[exp(km*c) exp(-km*c); km*exp(km*c) -km*exp(-km*c)];
    m45=m4*inv(m5);
m45 = [cosh(km*L) (-1/km)*sinh(km*L); -km*sinh(km*L) cosh(km*L)];
else
    m45=[1 -L; 0 1];
end

m67=m6*inv(m7);
m67=[cosh(p*w2) (-1/p)*sinh(p*w2); -p*sinh(p*w2) cosh(p*w2)];

M=inv(ml)*m23*m45*m67*m8; %[A;B]=M*[J;K]

M1=[1 -M(3); 0 -M(4)];
M2=[0 M(1); -1 M(2)];
S=inv(M2)*M1; %Scattering matrix relates incoming to outgoing amplitudes
%[B;J]=S*[A;K]
T=abs(S(2))^2;
%resdens.m
%created 24/7/01
%last modified 26/7/01
%written by Shanna Crankshaw

%finds the electron density \( n(k) \) inside the well for one value of \( V_m \)

\[
\text{m32} = \text{m3} \cdot \text{inv(m2)};
\]
\[
\text{m32} = \begin{bmatrix} \cosh(q \cdot w_1) & (1/q) \cdot \sinh(q \cdot w_1) \\ q \cdot \sinh(q \cdot w_1) & \cosh(q \cdot w_1) \end{bmatrix};
\]

\[
\text{if } E > V_m
\]
\[
\text{km} = \sqrt{2 \cdot m \cdot (E - V_m) / \hbar^2};
\]
\[
\text{m4} = \begin{bmatrix} \exp(i \cdot km \cdot b) & \exp(-i \cdot km \cdot b) \\ i \cdot km \cdot \exp(i \cdot km \cdot b) & -i \cdot km \cdot \exp(-i \cdot km \cdot b) \end{bmatrix};
\]
\[
\text{mu} = \text{inv(m4)} \cdot \text{m32} \cdot \text{m1};
\]
\[
\text{Mu} = \text{mu} \cdot [1; S(1)];
\]
\[
\text{F} = \text{Mu}(1); \quad \text{G} = \text{Mu}(2);
\]
\[
\text{n} = \text{L} \cdot (\text{abs(F)})^2 + \text{L} \cdot (\text{abs(G)})^2 + ((\text{F} \cdot \text{conj(G)})/(2 \cdot i \cdot \text{km})) \cdot (\exp(2 \cdot i \cdot \text{km} \cdot c) - \exp(2 \cdot i \cdot \text{km} \cdot b))
\]
\[
- ((\text{conj(F)} \cdot \text{G})/(2 \cdot i \cdot \text{km})) \cdot (\exp(-2 \cdot \text{km} \cdot c) - \exp(-2 \cdot \text{km} \cdot b));
\]

\[
\text{elseif } E < V_m
\]
\[
\text{km} = \sqrt{2 \cdot m \cdot (V_m - E) / \hbar^2};
\]
\[
\text{m4} = \begin{bmatrix} \exp(km \cdot b) & \exp(-km \cdot b) \\ km \cdot \exp(km \cdot b) & -km \cdot \exp(-km \cdot b) \end{bmatrix};
\]
\[
\text{mu} = \text{inv(m4)} \cdot \text{m32} \cdot \text{m1};
\]
\[
\text{Mu} = \text{mu} \cdot [1; S(1)];
\]
\[
\text{F} = \text{Mu}(1); \quad \text{G} = \text{Mu}(2);
\]
\[
(2 \cdot \text{km}) \cdot (\exp(-2 \cdot \text{km} \cdot c) - \exp(-2 \cdot \text{km} \cdot b)); (2 \cdot \text{km}) \cdot (\exp(2 \cdot \text{km} \cdot c) - \exp(2 \cdot \text{km} \cdot b)) - (\text{abs(G)})^2 /
\]

\[
\text{else}
\]
\[
\text{m4} = \begin{bmatrix} b & 1; 1 & 0 \end{bmatrix};
\]
\[
\text{mu} = \text{inv(m4)} \cdot \text{m32} \cdot \text{m1};
\]
\[
\text{Mu} = \text{mu} \cdot [1; S(1)];
\]
\[
\text{F} = \text{Mu}(1); \quad \text{G} = \text{Mu}(2);
\]
\[
\text{n} = (1/3) \cdot (\text{abs(F)})^2 \cdot (c^3 - b^3) + (1/2) \cdot (\text{F} \cdot \text{conj(G)} + \text{conj(F)} \cdot \text{G}) \cdot (c^2 - b^2) + \text{L} \cdot (\text{abs(G)})^2;
\]
\[
\text{end}
\]
%resonantcomp.m
%written by Shanna Crankshaw
%last modified 26/07/01
%creates density vectors for inside the well
%calculates current

format long;
parameters

energyTl=[]; %initializes energy vectors
energyTr=[];
Tl=[]; %initializes transmission vectors
Tr=[];
nl=[]; %initializes density vectors
nr=[];

for E = Emin:Eincr:muL
    resonant;
    resdens;
    energyTl = [energyTl E];
    Tl = [Tl T];
    nl = [nl n];
end

Vll=V1; V2l=V2; w1l=w1; w2l=w2;
V2r=V1l; V1r=V2l; w2r=w1l; w1r=w2l;
V1=V1r; V2=V2r; w1=w1r; w2=w2r; %interchanges w1<->w2 and V1<->V2;
clear V1l V2l w1l w2l V1r V2r w1r w2r

a=0; b=a+w1; c=b+L; d=c+w2; %defines parameters for -k states

for E=Emin:Eincr:muR
    resonant;
    resdens;
    energyTr = [energyTr E];
    Tr = [Tr T];
    nr = [nr n];
end

energynl=energyTl;
energynr=energyTr;
lengthen; %makes energynl and energynr the same length
n=nl+nr;
parameters %resets parameters for calculation of next +k state
%lengthen.m
%last modified 18/07/01
%written by Shanna Crankshaw

% makes vectors energynl and energynr the same length
% pads the shorter density vector with zeros

if length(nl)>length(nr)
    nright = 0*nl;
    nright(1:length(nr)) = nr;
    for count=length(nr)+1:length(nl)
        nright(count) = 0;
    end
    nr = nright;
    clear nright
    energynr = energynl;
elseif length(nl)<length(nr)
    nleft = 0*nr;
    nleft(1:length(nl)) = nl;
    for count=length(nl)+1:length(nr)
        nleft(count) = 0;
    end
    nl = nleft;
    clear nleft
    energynl = energynr;
else
    nl=nl;
    nr=nr;
end
%nvsrm.m
%last modified 26/07/01
%written by Shanna Crankshaw

%calculates the total integrated density for many different Vm values
%calculates the total integrated current for many different Vm values

parameters %sets barrier parameters
muL=Emin+500*Eincr %defines electrochemical potentials
muR=Emin+400*Eincr

Vmvalues = 10*qe*(0:.0001:.33); %defines vector of Vm (well hgt) values
dens = zeros(length(Vmvalues,(max(muL,muR)-Emin)/incr+1);

for counter = 1:length(Vmvalues),
    Vm=Vmvalues(counter);
    counter
    resonantcomp;
    Nlvalues(counter) = trapz(energynl,nl); %integrates n for +k states
    Nrvalues(counter) = trapz(energynr,nr); %integrates n for –k states
    Jlvalues(counter) = trapz(energyTl,Tl); %calc. current from +k states
    Jrvalues(counter) = trapz(energyTr,Tr); %calc. current from +k states
    dens(counter,: ) = n; %defines density matrix for single Vm
end

N=Nlvalues+Nrvalues; %total density
J=Jlvalues+Jrvalues; %net current
REFERENCES

